1,1,1,3,3,3-Hexafluoro-2-propanol

920-66-1 | DTXSID1022134

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 104 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.71e-01

Confidence level: 4.79e-01

Nearest Neighbors from the Training Set

Image not found
1-Decene
Measured: 159
Predicted: 1.31

Image not found
Ethane, 1,1-dichloro-1,2,2,2-tetrafluoro-
Measured: 33.1
Predicted: 2170

Image not found
Ethylene sulfide
Measured: 46.1
Predicted: 166

Image not found
Chloral
Measured: 71.3
Predicted: 41.1

Image not found
2-Methyl-2-butanol
Measured: 110
Predicted: 9.41